

Reply to Comment on "Reappraisal of the Electric Dipole Moment Enhancement Factor for Thallium"

H. S. Nataraj¹, B. K. Sahoo², B. P. Das³, and D. Mukherjee⁴

¹ *Cyclotron and Radioisotope Center, Tohoku University, 9808578 Sendai, Japan*

² *Theoretical Physics Division, Physical Research Laboratory, Ahmedabad 380009, India*

³ *Theoretical Astrophysics Group, Indian Institute of Astrophysics, 560034 Bangalore, India and*

⁴ *Indian Association for the Cultivation of Sciences, 700032 Kolkata, India*

In a recent Comment [arXiv:1108.3399], Dzuba and Flambaum have referred to the disagreement of the results of our latest calculations of Tl electron and scalar-pseudoscalar (S-PS) electric dipole moments (EDMs) and Cs parity non-conservation (PNC) with some other calculations. We have responded to all their points and also discussed the larger issues related to them. We have attempted to find the reasons for the disagreement between the results of our calculations and those of others. In particular, we have found that the two important reasons for the discrepancies between the Tl EDM calculations of Dzuba and Flambaum and ours are the different choice of single particle orbitals and the treatment of the valence-core correlation effects. We have demonstrated by numerical calculations that the V^{N-3} orbitals used by Dzuba and Flambaum overestimate the Tl electron and S-PS EDMs at the Dirac-Fock level. The failure of their suggested consistency test as interpreted by us is explained for systems with strong correlation like Tl. Also, the importance of understanding the physics underlying different theories on which atomic EDM and PNC calculations are based and comparisons between them are emphasized.

In their Comment [1], Dzuba and Flambaum begin by pointing out that our result for the electron EDM enhancement factor for Tl [2] is in disagreement with their calculation [3] as well as Liu and Kelly's [4]. They then go on to state with reference to our paper where this result was reported that "This is one more paper by this group presenting results which disagree with all other calculations. Others include, e.g. the calculations of the Tl EDM due to scalar-pseudoscalar (SPS) CP-odd interaction and parity nonconservation (PNC) in Cs." In this Comment, they do not, however, make any mention of our Cs EDM calculations based on the relativistic coupled-cluster (RCC) theory [5] which agrees well with their calculations [3]. With reference to this agreement, Dzuba and Flambaum had stated in their paper [3] that "Our calculations are in good agreement with the most recent and accurate calculations". The reference that they had given for the most recent and accurate calculations was our Cs EDM work [5]. Furthermore, they do not refer to our Ba⁺ and Ra⁺ PNC papers [6, 7] in their Comment. In a recent paper Dzuba and Flambaum [8] have reported that our Ba⁺ and Ra⁺ PNC results are in agreement with those of their latest calculations.

We feel it is necessary to put the above remarks of Dzuba and Flambaum on our Tl EDM and Cs PNC calculations in perspective. A large number of calculations of the electron EDM enhancement factor (EDM-EF) for Tl have been performed using a variety of methods over the past four decades. We have mentioned in our paper [2] that the results of these calculations vary from -179 to -1041 . This is also evident from Dzuba and Flambaum's paper [3]. The reason for this variation is the peculiarly large electron correlation effects in Tl EDM-EF. While it is true that our result does not agree with those of other calculations which were carried out using approximations substantially different from ours, it

is equally true that the result of Dzuba and Flambaum agrees well with only the calculation of Liu and Kelly [4]. As we have explained in our paper [2] this agreement is fortuitous. In their paper [3], Dzuba and Flambaum simply state this agreement, without giving any reasons for it. In contrast, we [2] have endeavoured to explain the discrepancies between our results and those of Liu and Kelly [4] and Dzuba and Flambaum [3]. For any scientific problem, the mere agreement or disagreement between two results is far less important than the reasons underlying them. It is therefore imperative to try to understand these reasons when one is comparing the results of two different theoretical methods. As for the differences between Liu and Kelly's work and ours, we reiterate the following points that we had stated in our paper [2]: "The following approximations were made in the former work (Liu and Kelly) (i) An approximation to only the one electron part of the EDM Hamiltonian is considered, thereby neglecting the important contributions partly from the DF potential and largely from the two electron Coulomb interaction. (ii) Only the linear terms and a few selected nonlinear terms have been used in the calculations. The CC equations have not been fully solved even at the CCSD level as a coupled-electron pair approximation has been used to solve for the quadratic terms that have been taken in the unperturbed doubles equation. (iii) A few selected triple excitations are included only in the unperturbed singles amplitude equations, where as, several dominant triples terms are completely ignored in the unperturbed doubles equations. Thus, the contribution of triples is taken into account in a nonstandard way. (iv) The inner core is frozen up to the 4s orbital for the calculation of the unperturbed amplitudes, where as, for solving the perturbed doubles equations, 4s, 4p and 4d orbitals are further frozen. Such an inconsistent treatment introduces uncontrollable er-

rors. In contrast to the above drawbacks, we consider all the nonlinear terms arising from the single and double excitations. In addition, we consider the leading triple excitations in both the unperturbed singles and doubles cluster equations. We solve the unperturbed and perturbed, closed- and open-shell equations, self consistently in the framework of the relativistic CCSD(T) approach, taking into account the excitations from all the core electrons."

It is evident from the above comparison that Dzuba and Flambaum's point in their Comment [1] that Liu and Kelly have used the same relativistic coupled cluster method that we have used to calculate the EDM-EF for Tl is extremely specious. It makes very little sense for us to spend a few months to try and reproduce their result, particularly when we know that it is based on inconsistent approximations leading to cluster amplitudes that are partially unphysical. Given these shortcomings of Liu and Kelly's work, a better way of testing the reliability of our Tl EDM-EF calculation would be to compare the results of our calculated quantities like allowed electric dipole transition amplitudes and hyperfine constants that are related to the EDM enhancement factor with available experimental data. That is precisely what we have done in Table IV of our paper [2]. The overall agreement of our calculations with measurements is better than that of Dzuba and Flambaum [3]. Liu and Kelly [4] have not performed any of these calculations. We are surprised that Dzuba and Flambaum have not referred at all to the comparison of the calculations of the relevant Tl transition amplitude and hyperfine constants in their Comment [1]. While these properties for Tl are not as sensitive to electron correlation effects as the EDM-EF, it is necessary to calculate them in order to get a sense of their accuracies as they are related to the EDM-EF.

With reference to our comments about the comparison between Dzuba and Flambaum and our calculations in our paper [2], we would like to categorically state that they are not misleading. We had not made any claims about the P and T violating Hamiltonian that Dzuba and Flambaum had used. Rather, we had surmised the form of their Hamiltonian as they had not given any information about it in their paper. In order to clarify, we reproduce the relevant excerpt from our paper: "It appears from the previous work of Dzuba and Flambaum that the P & T violating Hamiltonian used in [10], considers only the internal electric field due to the nucleus and not the electrons; i.e., the entire two body Coulomb potential is neglected." It is still not clear to us from Dzuba and Flambaum's Comment [3], whether they have included the gradient of the exact or the approximate two-electron Coulomb potential—they have not given the explicit form of their Hamiltonian.

Indeed, we did mention in our paper that the V^{N-3} core, virtual and valence orbitals of Dzuba and Flambaum are highly contracted—plots of some of these orbitals are given in Figs. (a)-(f). We should have worded it more carefully and emphasized that the V^{N-3} valence

($6p_{1/2}$) and the virtual (7s) orbitals are highly contracted at large r relative to their V^{N-1} counterparts as shown in Figs. (d) and (f). The EDM-EF for Tl is very sensitive to the choice of $6p_{1/2}$, 7s and 6s orbitals and it is clearly desirable to use V^{N-1} orbitals for an accurate determination of this quantity as they exhibit the correct physical behaviour, particularly at large r unlike the V^{N-3} orbitals.

Table I highlights the large discrepancies between the V^{N-1} and V^{N-3} Dirac-Fock (DF) results for Tl EDM-EF and related properties. In retrospect, it appears that this is an important reason for the disagreement between the results of Dzuba and Flambaum [3] and our [2] calculations. The V^{N-3} RCC result for Tl EDM-EF would be -560 if one assumes that it changes in the same proportion to the DF as it does in the V^{N-1} case. This of course is not a rigorous assumption. It would not be out of place to mention here that in view of our DF results for the two kinds of orbitals, the agreement between the CI+MBPT result of Dzuba and Flambaum [3] with V^{N-3} orbitals and that of the linearized RCC calculation of Liu and Kelly [4] with V^{N-1} orbitals does indeed appear to be fortuitous as we had remarked earlier based on other considerations.

TABLE I: Various results for different orbitals obtained using V^{N-3} and V^{N-1} potentials in Tl.

States/Transitions	V^{N-1}	V^{N-3}
<u>Enhancement factors due to d_e</u>		
$6p_{1/2}$	-422.02	-507.15
<u>S-PS ratio in unit given in [9]</u>		
$6p_{1/2}$	5.02	6.04
<u>Energy difference in cm^{-1}</u>		
$6p_{1/2} - 6s$	107507.67	60294.73
$6p_{1/2} - 7s$	22714.75	67140.58
<u>Reduced E1 elements in au</u>		
$6p_{1/2} - 6s$	2.08	2.02
$6p_{1/2} - 7s$	2.05	1.26
<u>Matrix element of H_{EDM}^{de}</u>		
$6p_{1/2} - 6s$	44.26	60.89
$6p_{1/2} - 7s$	10.37	29.61

It is clear from Table I of our paper [2] that there are delicate cancellations between various valence-core correlations that we have evaluated to all orders using the RCC method in the singles, doubles and partial triples approximation. Dzuba and Flambaum [3] have calculated some of these effects (Brueckner pair correlation) mainly by second order many-body perturbation theory and have neglected some others like structural radiation

and different classes of higher order RCC terms. The combined contributions from the latter two effects to Tl EDM-EF are about 30; which is by no means negligible. The approximations used in [3] to calculate the valence-core correlations will not be able to capture the cancellations in our all order RCC calculations.

We now turn to the S-PS EDM calculations for Tl. Three relativistic many-body calculations have been carried out for this quantity [3, 9, 10]. Dzuba and Flambaum's calculation agrees with that of Martensson-Pendrill and Lindroth [10], even though the approximations used in the calculations are quite different. The latter work considers one electron effects to all orders, but its treatment of the two electron correlation effects is rather approximate. It only takes into account the Brueckner pair correlation which is not calculated directly, but rather it is estimated on the basis of its contribution to the electron EDM-EF of Tl from Hartley et al's work [11], which had been performed using the same method that Martensson-Pendrill and Lindroth had used in their S-PS EDM calculation [10]. Therefore, the latter calculation is somewhat less reliable than the former. The S-PS EDM calculations of Dzuba and Flambaum and Martensson-Pendrill and Lindroth agree, but the electron EDM-EF calculation of the former is more than three times larger than that of the latter. This is indeed mind boggling and therefore one cannot attach any importance to the agreement of the Tl S-PS EDM results of the two sets of authors. Dzuba and Flambaum have not given any explanation for this paradoxical situation. We had employed the RCC method in the singles, doubles and partial triples approximation [9] and it is therefore not at all surprising that our calculation does not agree with the other two calculations which are based on different approximations.

Dzuba and Flambaum [1] begin the last paragraph of their Comment by asserting that our Tl EDM-EF [2] and S-PS EDM [9] calculations do not satisfy a simple consistency test. However, they conclude by making a rather tentative statement that these two calculations may be internally inconsistent. The consistency test in their own words [1] is as follows: "the ratio of the EDMs due to two operators must be approximately equal to the ratio of the sp single-electron matrix elements of these operators. This is because only short distances, where single-electron energies can be neglected, contribute to the single-electron matrix elements of the CP-odd operators." We do not fully understand what this test is supposed to mean. Which s-p single electron matrix elements are they referring to? 6s-6p1/2 or 7s-6p1/2 or something else? They have not been very specific. Perhaps the meaning would have been clearer if they had supplemented what they have written by mathematical expressions. Towards the end of their Comment [1], Dzuba and Flambaum seem to suggest that our value for the ratio they have mentioned in their consistency test is $115 d_e/C^{SP} 10^{18} \text{ ecm}$ and not $89 d_e/C^{SP} 10^{18} \text{ ecm}$, which they probably think is the correct value. The for-

mer is the value of the ratio of the electron EDM-EF to the S-PS EDM for Tl that we have got at the RCC level [2, 9] and our value for the same ratio at the DF level is $84 d_e/C^{SP} 10^{18} \text{ ecm}$. It therefore appears that the consistency test that they have referred to in the context of our calculations means our ratios of the values of the two EDMs for the RCC and DF cases should be approximately equal. In other words, the ratio of the of electron EDM-EFs of the RCC and DF calculations is approximately equal to the the ratios of the atomic EDM to the S-PS constant for the same two methods. If our interpretation is correct then it is straightforward to show that the test that they have proposed does not hold in general, and in particular, we shall explain why it fails for Tl. In order to do so, we begin with the unperturbed and first order perturbed wave functions in the RCC approach which can be expressed as [2, 9]

$$|\Psi_v^{(0)}\rangle = e^{T^{(0)}} \{1 + S_v^{(0)}\} |\Phi_v\rangle, \quad \text{and} \quad (1)$$

$$|\Psi_v^{(1)}\rangle = e^{T^{(0)}} \{T^{(1)} (1 + S_v^{(0)}) + S_v^{(1)}\} |\Phi_v\rangle \quad (2)$$

respectively, and the electron EDM enhancement factor or in general the ratio of the atomic EDM to a CP violating coupling constant is given by the exact expression

$$\begin{aligned} \mathcal{R} &= \langle \Psi_v^{(0)} | D | \Psi_v^{(1)} \rangle + \langle \Psi_v^{(1)} | D | \Psi_v^{(0)} \rangle \\ &= [\langle \Phi_v | \bar{D}^{(0)} T^{(1)} + \bar{D}^{(0)} S_v^{(1)} + \bar{D}^{(0)} T^{(1)} S_v^{(0)} \\ &\quad + S_v^{(0)\dagger} \bar{D}^{(0)} T^{(1)} + S_v^{(0)\dagger} \bar{D}^{(0)} S_v^{(1)} \\ &\quad + S_v^{(0)\dagger} \bar{D}^{(0)} T^{(1)} S_v^{(0)} | \Phi_v \rangle] + hc \\ &= \mathcal{R}_1 + \mathcal{R}_2 + \mathcal{R}_3 + \mathcal{R}_4 + \mathcal{R}_5 + \mathcal{R}_6, \end{aligned} \quad (3)$$

with $\bar{D}^{(0)} = e^{T^{(0)\dagger}} D e^{T^{(0)}}$ and each term along with its hermitian conjugate (hc) term is given with subscripts from 1 to 6 with their sequence. To define the single and double excitations, we use the subscripts 1 and 2 for all the RCC operators (for the detail see [2, 9]). As mentioned in [2, 13], the core and virtual contributions at the DF level comes at the lowest order through the RCC terms $\langle \Phi_v | \bar{D}^{(0)} T^{(1)} | \Phi_v \rangle$ and $\langle \Phi_v | \bar{D}^{(0)} S_v^{(1)} | \Phi_v \rangle$, respectively. Denoting $\mathcal{R}_1 = \mathcal{R}_c^{DF} + \mathcal{R}_1^{corr}$ and $\mathcal{R}_2 = \mathcal{R}_v^{DF} + \mathcal{R}_2^{corr}$, the total DF result is given by $\mathcal{R}_{DF} = \mathcal{R}_c^{DF} + \mathcal{R}_v^{DF}$. With these notations, the above expression can be rewritten as

$$\begin{aligned} \frac{\mathcal{R}}{\mathcal{R}_{DF}} &= 1 + \frac{\mathcal{R}_1^{corr}}{\mathcal{R}_{DF}} + \frac{\mathcal{R}_2^{corr}}{\mathcal{R}_{DF}} + \frac{\mathcal{R}_3}{\mathcal{R}_{DF}} + \frac{\mathcal{R}_4}{\mathcal{R}_{DF}} \\ &\quad + \frac{\mathcal{R}_5}{\mathcal{R}_{DF}} + \frac{\mathcal{R}_6}{\mathcal{R}_{DF}}. \end{aligned} \quad (4)$$

All the terms on the right hand side of the above equation are built out of different combinations of D , $T^{(0)}$, $S_v^{(0)}$, $T^{(1)}$, and $S_v^{(1)}$. The last two operators; i.e. $T^{(1)}$ and $S_v^{(1)}$ contain one order of the EDM interaction and all orders in the residual Coulomb interaction. The electron EDM interaction Hamiltonian is given by

$$H_{EDM}^e = 2icd_e \sum_j \beta_j \gamma_j^5 p_j^2 \quad (5)$$

and the S-PS interaction Hamiltonian is given by

$$H_{EDM}^{S-PS} = \frac{iG_F}{\sqrt{2}} C_S \sum_j \beta_j \gamma_j^5 \rho_{nuc}^j(r), \quad (6)$$

where d_e is the intrinsic e -EDM, γ^5 is a pseudo-scalar Dirac matrix, C_S is the dimensionless S-PS constant and $\rho_{nuc}^j(r)$ is the j th electron density over the nucleus. The corresponding single particle electron EDM and the S-PS matrix elements are given by

$$\begin{aligned} \langle \phi_i || h_{EDM}^e || \phi_j \rangle &= -2c\sqrt{2j_i+1}\delta(\kappa_i, -\kappa_j) \\ &\quad \int_0^\infty dr \left(\frac{\tilde{l}_j(\tilde{l}_j+1)}{r^2} P_i(r) Q_j(r) \right. \\ &\quad \left. + \frac{l_j(l_j+1)}{r^2} Q_i(r) P_j(r) \right. \\ &\quad \left. + \frac{dP_i}{dr} \frac{dQ_j}{dr} + \frac{dQ_i}{dr} \frac{dP_j}{dr} \right) \end{aligned} \quad (7)$$

and

$$\begin{aligned} \langle \phi_i || h_{EDM}^{S-PS} || \phi_j \rangle &= \frac{G_F}{\sqrt{2}} C_S \sqrt{2j_i+1} \delta(\kappa_i, -\kappa_j) \\ &\quad \int_0^\infty dr (P_i(r) Q_j(r) \\ &\quad + Q_i(r) P_j(r)) \rho_{nuc}^j(r), \end{aligned} \quad (8)$$

respectively, where l and \tilde{l} are the orbital quantum numbers for the large and small components of the Dirac orbitals. It is clear that the above two matrix elements are numerically quite different, even though both of them are large in the nuclear region. The amplitudes for $T^{(1)}$, and $S_v^{(1)}$ are therefore different for the two EDMs; particularly in Tl where the electron correlation effects are strong. This is because these amplitudes represent different processes involving the EDM and the correlation effects. Therefore $\frac{\mathcal{R}}{\mathcal{R}_{DF}}$ would in general be different for the electron EDM and the S-PS interaction making the consistency test that Dzuba and Flambaum have suggested invalid for systems with large correlation effects; although it could hold in situations when the correlation effects are weak or moderately strong. This is reflected in the results of our RCC calculations of the two EDMs for Tl—see the relevant tables [2, 13]. The trends exhibited by some of the RCC terms in the two cases are different—the most striking being the relative contributions of $DT^{(1)}$ and $DS_v^{(1)}$. As a result, the relative contributions of $\frac{\mathcal{R}_1^{corr}}{\mathcal{R}_{DF}}$ and $\frac{\mathcal{R}_2^{corr}}{\mathcal{R}_{DF}}$ are quite different.

We would now like to clarify certain issues related to our parity nonconservation (PNC) calculation in Cs that the Dzuba and Flambaum [1] have commented on. It is certainly not true that our Cs PNC result does not agree with the results of other calculations of this quantity. In an earlier work, we had reported our Cs PNC result as $0.902(4) \times 10^{-11} iea_0 - Q_W/N$ from a preliminary calculation [12] and more recently we obtained $0.8892 \times$

$10^{-11} iea_0 - Q_W/N$ (triple excitations involving the valence and two core electrons were incorporated in the latest result) [13] using the RCC method. The latter result is in agreement with another recent calculation by Porsev et al [14], who have got $0.8891 \times 10^{-11} iea_0 - Q_W/N$ in the framework of the Dirac-Coulomb approximation using unscaled wave functions by a sum-over-states relativistic coupled-cluster (CC) method at the singles, doubles and leading order triple excitations which is at par with our approach. However, Porsev et al have minimized the uncertainty in the calculation by scaling the wave functions and they have added other corrections to get the final result. They have used their final result to probe new physics. In our work, we have only demonstrated the important role of correlation effects using an *ab initio* RCC method and we have not put any effort to minimise the uncertainty at the Dirac-Coulomb level or considered higher order relativistic and nuclear corrections to probe new physics using our results. Our result is not in serious conflict with any other calculation if it is viewed in the right context. The reported results of Dzuba and Flambaum are $0.9001 \times 10^{-11} iea_0 - Q_W/N$ [15] and $0.9078 \times 10^{-11} iea_0 - Q_W/N$ [16] at the Dirac-Coulomb approximation. The same authors had also reported the s-d PNC amplitude calculations in Ba^+ and Ra^+ [17] about a decade ago [17]. They had obtained 2.17 and 2.37 (in $\times 10^{-11} iea_0 - Q_W/N$) for Ba^+ and 42.9 and 45.9 (in $\times 10^{-11} iea_0 - Q_W/N$) for Ra^+ using a mixed state and the sum-over-states approaches, respectively. In their Comment, the same authors had expressed the view that it is necessary to obtain accurate results for these calculations in order to use them for inferring new physics [1]. But their dual results could not have been useful for this purpose. Accurate PNC results for these ions were only identified when we employed the RCC method and reported our results as 2.46(2) and 46.4(1.4) (in $\times 10^{-11} iea_0 - Q_W/N$) for Ba^+ [6] and Ra^+ [7], respectively. We learnt from a recent work of Dzuba and Flambaum that using one of their advanced methods, they were able to improve their results to 0.29 and 3.4 (in $\times 10^{-12} iea_0 - Q_W$) [3] compared with our results 0.304 and 3.33 (in $\times 10^{-12} iea_0 - Q_W$) in Ba^+ and Ra^+ , respectively. We quote below from their paper [8]: "There is also good agreement with Sahoo *et al.* for Ba^+ [21] and with Wansbeek *et al.* for Ra^+ [17]".

In conclusion, we have responded to all the points raised by Dzuba and Flambaum in their Comment [1] on our Tl EDM and Cs PNC calculations. The reasons for the discrepancies between Liu and Kelly [4] and our calculations which were discussed in our paper [2] have been reiterated. The two main reasons for the disagreement between Dzuba and Flambaum and our Tl EDM calculations have been identified as the choice of orbitals (V^{N-3} by Dzuba and Flambaum and V^{N-1} by us) and the treatment of valence-core correlation.

It has been pointed out that the agreement of the Tl electron EDM results of Liu and Kelly and Dzuba and Flambaum is fortuitous. We have provided strong evi-

dence to show that the agreement of the Tl S-PS EDM results of Dzuba and Flambaum [3] and Martensson-Pendrill and Lindroth [10] raises many more questions than it answers. We have argued that the consistency test that Dzuba and Flambaum have referred to in their Comment involving the electron and S-PS EDMs as interpreted by us is flawed. Our RCC results for quantities that are associated with Tl EDM are in better agreement with experimental data than those of Dzuba and Flambaum, which these two authors do not mention in their Comment. Contrary to the comments made by Dzuba and Flambaum on our Cs PNC work, our result does agree with that of another calculation that was performed at the same level of approximation [14].

Dzuba and Flambaum refer to three calculations (Tl electron EDM, Tl S-PS EDM and Cs PNC) in their Comment for which their results are different from ours. However, in the same Comment, they do not mention the re-

sults of our Cs electron EDM, Cs S-PS EDM, Ba^+ PNC and Ra^+ PNC calculations which are in agreement with theirs. When the result of a calculation of ours agrees with theirs as in the case of Cs EDM [5], it is described as accurate by them [3], but on the other hand if it does not agree then they make adverse remarks against it as exemplified in their Comment [1]. Dzuba and Flambaum have not made any attempt to explain why a particular result agrees or disagrees with their result [1, 3]— they have merely stated whether it agrees with their result or not. Such an approach provides no insights into the reasons for the agreement or disagreement between the two methods that were used to obtain these results. An understanding of the physics embodied by the methods used in the calculations of atomic EDMs and PNC and comparisons between them are prerequisites for making further progress in this field.

-
- [1] V. A. Dzuba and V. V. Flambaum, arXiv:1108.3399.
 - [2] H. S. Nataraj, B. K. Sahoo, B. P. Das and D. Mukherjee, Phys. Rev. Lett. **106**, 200403 (2011).
 - [3] V. A. Dzuba and V. V. Flambaum, Phys. Rev. A **80**, 062509 (2009).
 - [4] Z. W. Liu and H. P. Kelly, Phys. Rev. A **45**, R4210 (1992).
 - [5] H. S. Nataraj, B. K. Sahoo, B. P. Das and D. Mukherjee, Phys. Rev. Lett. **106**, 033002 (2008).
 - [6] B. K. Sahoo, R. K. Chaudhuri, B. P. Das and D. Mukherjee, Phys. Rev. Lett. **96**, 163003 (2006).
 - [7] L. W. Wansbeek, B. K. Sahoo, R. G. E. Timmermans, B. P. Das and D. Mukherjee, Phys. Rev. A **78**, 012515(R) (2008).
 - [8] V. A. Dzuba and V. V. Flambaum, Phys. Rev. A **83**, 052513 (2011).
 - [9] B. K. Sahoo, B. P. Das, Rajat K. Chaudhuri, Debashis Mukherjee and E. P. Venugopal, Phys. Rev. A **78**, 010501(R) (2008).
 - [10] A. -M. Mårtensson-Pendrill and E. Lindroth, Eur. Phys. Lett. **15**, 155 (1991).
 - [11] A. C. Hartley, E. Lindroth and A. -M. Martensson-Pendrill, J. Phys. B **23**, 3417 (1990).
 - [12] B. P. Das, B. K. Sahoo, G. Gopakumar and R. K. Chaudhuri, J. Mol. Structure: THEOCHEM **768** 141 (2006).
 - [13] B. K. Sahoo, J. Phys. B **43**, 085005 (2010).
 - [14] S. G. Porsev, K. Beloy and A. Derevianko, Phys. Rev. D **82**, 036008 (2010).
 - [15] V. A. Dzuba, V. V. Flambaum and M. S. Safronova, Phys. Rev. A **73**, 022112 (2006).
 - [16] V. A. Dzuba, V. V. Flambaum and J. S. M. Ginges, Phys. Rev. D **66**, 076013 (2002).
 - [17] V. A. Dzuba, V. V. Flambaum and J. S. M. Ginges, Phys. Rev. A **63**, 062101 (2001).

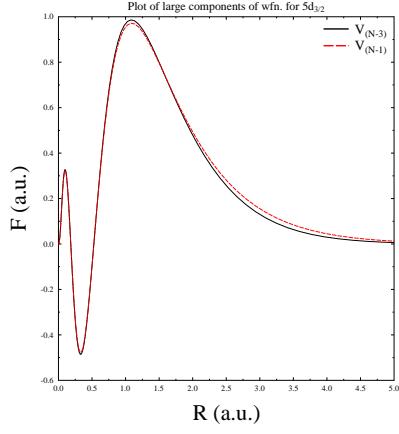
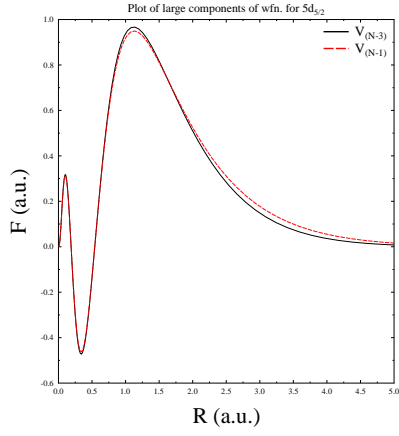
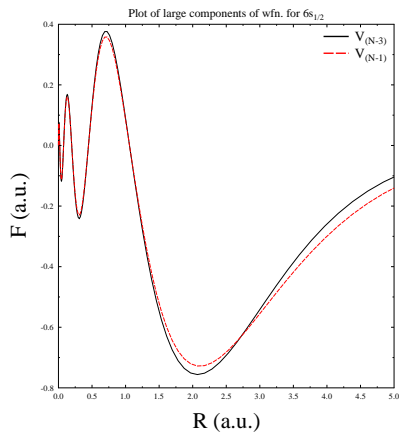
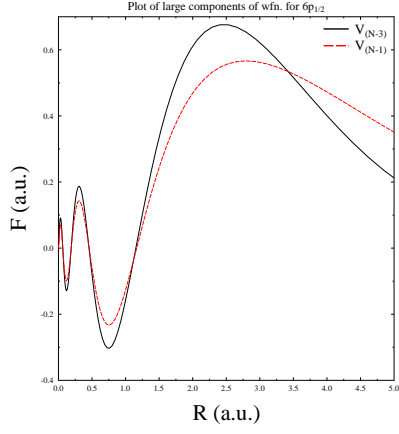
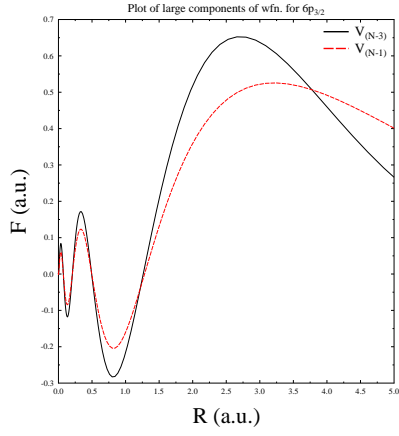
(a) $5d_{3/2}$ orbital wave function(b) $5d_{5/2}$ orbital wave function(c) $6s_{1/2}$ orbital wave function

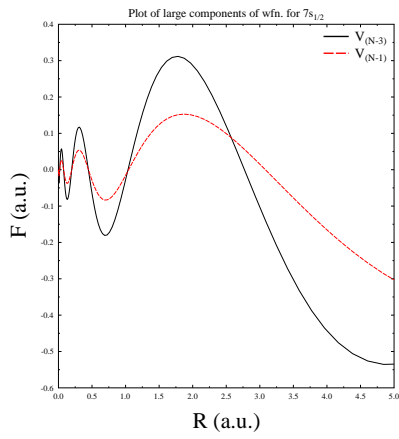
FIG. 1: Comparison of magnitudes of the $5d_{3/2}$, $5d_{5/2}$, and $6s_{1/2}$ single particle wave functions using V^{N-3} and V^{N-1} potentials.



(d) $6p_{1/2}$ orbital wave function



(e) $6p_{3/2}$ orbital wave function



(f) $7s_{1/2}$ orbital wave function

FIG. 2: Comparison of magnitudes of the $6p_{1/2}$, $6p_{3/2}$, and $7s_{1/2}$ single particle wave functions using V^{N-3} and V^{N-1} potentials.